

Upper bounds on the Laplacian energy of some graphs

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Abstract

The Laplacian energy $(LE)_G$ of a simple graph G with n vertices and m edges is equal to the sum of distances of the Laplacian eigenvalues to their average, which in turn is equal to the sum of singular values of $L(G) - \frac{2m}{n} I_n$, namely of a shift of the Laplacian matrix of G . For $1 \leq j \leq s$, let A_j be matrices of orders n_j . Suppose that

$$\det(L(G) - \lambda I_n) = \prod_{j=1}^s \det(A_j - \lambda I_{n_j})^{t_j}.$$

In the present paper we prove

$$(LE)_G \leq \sum_{j=1}^s t_j \sqrt{n_j} \|A_j - \frac{2m}{n} I_{n_j}\|_F \leq \sqrt{n} \|L(G) - \frac{2m}{n} I_n\|_F,$$

where $\|\cdot\|_F$ stands for the Frobenius matrix norm.

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1 Preliminaries

Let $G = (V, E)$ be a simple (n, m) -graph where V is a nonempty finite set of n vertices and E is the set of m edges. We denote by $d_1 \geq \dots \geq d_n$ its vertex degree sequence. Let $D(G)$ be the diagonal matrix of vertex degrees and $A(G)$ the adjacency matrix. Its eigenvalues $\lambda_1, \dots, \lambda_n$ form the spectrum of G . The matrix $L(G) = D(G) - A(G)$ is the Laplacian matrix of G . The Laplacian spectrum of G corresponds to eigenvalues μ_1, \dots, μ_n of $L(G)$, (cf. [1]).

The notion of energy of a (n, m) -graph G (written $(E)_G$) was introduced by Gutman and it is intensively studied in chemistry since it can be used to approximate the total π -electron energy of a molecule (cf. [3],[4],[5] and [8]).

It is defined by

$$(E)_G = \sum_{j=1}^n |\lambda_j|,$$

whereas the Laplacian energy of a (n, m) -graph G (written $(LE)_G$) (cf. [6], [7]) is defined by

$$(LE)_G = \sum_{j=1}^n \left| \mu_j - \frac{2m}{n} \right|. \quad (1)$$

Given a complex $m \times n$ matrix C , we index its singular values by $s_1(C), s_2(C), \dots$.

The value

$$\mathcal{E}(C) = \sum_j s_j(C),$$

is the energy of C (cf.[10]), thereby extending the concept of graph energy introduced by Gutman. Consequently, if $C \in \mathbb{R}^{n \times n}$ is symmetric with eigen-

values $\lambda_1(C), \dots, \lambda_n(C)$ its energy is given by

$$\mathcal{E}(C) = \sum_{i=1}^n |\lambda_i(C)|.$$

Let $s \in \mathbb{N}$. Denote I_s the corresponding identity matrix of order s . Evidently, using the previous concept, the energy of any graph G is the energy of its adjacency matrix and its Laplacian energy is given by

$$(LE)_G = \mathcal{E}\left(L(G) - \frac{2m}{n}I_n\right). \quad (2)$$

Let $C = (c_{ij})_{1 \leq i, j \leq n}$ be a square matrix so that $\sigma(C)$ and $\|C\|_F$ denote the eigenvalues set (with its multiplicity) of C and the Frobenius matrix norm of C , [9], respectively. Moreover, consider the matrix $|C| = (C^T C)^{1/2}$. If C is a symmetric matrix, then the next formula relates the above definitions.

$$\begin{aligned} \|C\|_F &= \left(\sum_{i,j=1}^n |c_{ij}|^2 \right)^{1/2} \\ &= (\text{trace } |C|^2)^{1/2} \\ &= \left(\sum_{\lambda \in \sigma(C)} |\lambda|^2 \right)^{1/2}. \end{aligned}$$

The following upper bound on the energy of a (n, m) -graph G have been established, [6].

$$(E)_G \leq \sqrt{2mn}. \quad (3)$$

By setting

$$M = m + \frac{1}{2} \sum_{j=1}^n \left(d_j - \frac{2m}{n} \right)^2, \quad (4)$$

the authors, in [6], together with the concept of Laplacian energy introduced the next upper bound (analogous to (3)),

$$(LE)_G \leq \sqrt{2Mn}. \quad (5)$$

A standard verification shows that

$$2M = \left\| L(G) - \frac{2m}{n} I_n \right\|_F^2. \quad (6)$$

Thus Eq. (5) can be expressed by

$$(LE)_G \leq \sqrt{n} \left\| L(G) - \frac{2m}{n} I_n \right\|_F.$$

The aim of this paper is to establish a new and improved upper bound for the Laplacian energy of graphs whose Laplacian characteristic polynomial can be decomposed as a product of other characteristic polynomials. Moreover, we prove for the mentioned graphs that our new upper bound is better than (5).

There are numerous results in the literature related with the decomposition of the characteristic polynomial and the Laplacian polynomial. For example, in [11] Rojo and Soto have decomposed the characteristic polynomial and the Laplacian characteristic polynomial of generalized Bethe trees as a product of characteristic polynomial of nonnegative, symmetric, tridiagonals matrices [cf. [11], [12], and [13]]. Recently Fernandes R. et al, [2], also done a similar decomposition for graphs like weighted rooted trees. The authors also decomposed the characteristic polynomial as a product of characteristic polynomial of nonnegative, symmetric, tridiagonals matrices and some polynomials related with the characteristic polynomials of the referred matrices. As an application of our result, with the decompositions presented in [11] we construct an improved upper bound (in comparison with (5)) of the Laplacian energy to the case of generalized Bethe trees.

In order to state our result, we introduce the following notation. For $a = (a_1, \dots, a_q) \in \mathbb{R}^q$ its norm $\|a\|$, is given by $\|a\| = \sqrt{a_1^2 + a_2^2 + \dots + a_q^2}$. Let $b = (b_1, \dots, b_q) \in \mathbb{R}^q$. We recall the Cauchy Schwarz inequality (cf. [9]):

$$\sum_{j=1}^q a_j b_j \leq \|a\| \|b\|.$$

Let $p \leq q$. Define

$$W^p = \{a = (a_1, \dots, a_q) \in \mathbb{R}^q : a_{p+1} = \dots = a_q = 0\}.$$

It is well known that W^p is a subspace p dimensional of \mathbb{R}^q . For $a = (a_1, \dots, a_q) \in \mathbb{R}^q$ consider the vectors $\varepsilon_p(a) := (a_1, \dots, a_p, 0, \dots, 0) \in W^p$ and $\delta_p(a) := (a_{p+1}, \dots, a_q, 0, \dots, 0) \in W^{q-p}$.

The following properties can be directly verified:

1. $\delta_p(\varepsilon_p(a)) = (0, \dots, 0),$
2. $\delta_{p_1}(\delta_{p_2}(a)) = \delta_{p_1+p_2}(a)$ and
3. $\|a - \varepsilon_p(a)\|^2 = \|\delta_p(a)\|^2 = \|a\|^2 - \|\varepsilon_p(a)\|^2.$

Lemma 1 *Let $a = (a_1, \dots, a_q) \in \mathbb{R}^q$. Let $p \leq q$ and consider $\varepsilon_p(a)$ and $\delta_p(a)$ defined as above. Then,*

$$\sqrt{p} \|\varepsilon_p(a)\| + \sqrt{q-p} \|\delta_p(a)\| \leq \sqrt{q} \|a\|. \quad (7)$$

Proof. If $a = (0, \dots, 0) \in \mathbb{R}^q$ the inequality (7) is trivially verified. From now on we consider $a \neq 0$. Let $b = (b_1, \dots, b_q) \in \mathbb{R}^q$ be the unitary vector $\frac{a}{\|a\|}$ namely $b_i = a_i / \|a\|$, for $1 \leq i \leq q$. Thus,

$$\|\varepsilon_p(b)\|^2 = b_1^2 + b_2^2 + \dots + b_p^2 \leq 1$$

and

$$\|a\|^2 \|\varepsilon_p(b)\|^2 = \|\varepsilon_p(a)\|^2. \quad (8)$$

It is easily checked that the inequality (7) follows from the inequality

$$\sqrt{p} \|\varepsilon_p(b)\| + \sqrt{(1 - \|\varepsilon_p(b)\|^2)(q-p)} \leq \sqrt{q}, \quad (9)$$

together with Eq. (8) and the property **3**. Thus, this prove can be obtained from establish that

$$\sqrt{pg} + \sqrt{(1-g)(q-p)} \leq \sqrt{q} \text{ for all } 0 \leq g \leq 1. \quad (10)$$

On this way, we just use the fact that, the arithmetic mean of two non-negative real numbers is greater than or equal to the geometric mean of them. By the previous fact considering the nonnegative numbers qg and p we obtain, $2\sqrt{qg}\sqrt{p} \leq qg + p$. From this, we derive to $q - qg - p + pg \leq q + pg - 2\sqrt{q}\sqrt{pg}$. Then,

$$(q-p)(1-g) \leq (\sqrt{q} - \sqrt{pg})^2. \quad (11)$$

Now, by computing in both sides square root in inequality (11), the inequality (10) holds. Hence, by considering $g = \|\varepsilon_p(b)\|^2$ the inequality (9) follows. ■

Theorem 2 *Let A_j be square symmetric matrices of order n_j and $P_j(\lambda) = \det(A_j - \lambda I_{n_j})$ with $1 \leq j \leq s$. Consider a square symmetric matrix A of order n with characteristic polynomial $P(\lambda)$ so that*

$$P(\lambda) = P_1(\lambda)P_2(\lambda) \dots P_s(\lambda). \quad (12)$$

Then

$$\mathcal{E}(A) \leq \sum_{j=1}^s \sqrt{n_j} \|A_j\|_F \leq \sqrt{n} \|A\|_F. \quad (13)$$

Proof. From the statement it is clear that

$$n = \sum_{i=1}^s n_i.$$

Let $1 \leq j \leq s$ and $\sigma(A_j) = \{\mu_{ij} : 1 \leq i \leq n_j\}$, be the spectrum of A_j . Thus, $\sigma(|A_j|) = \{s_{ij} = |\mu_{ij}| : 1 \leq i \leq n_j\}$. Consider the vectors $\alpha_j = (s_{1j}, \dots, s_{n_j j}) \in \mathbb{R}^{n_j}$. From definition of Frobenius matrix norm we obtain

$$\|A_j\|_F^2 = \|\alpha_j\|^2 = \sum_{i=1}^{n_j} s_{ij}^2, \quad 1 \leq j \leq s.$$

With our notation, $a = (\alpha_1, \dots, \alpha_s)$ is the vector of eigenvalues of $|A|$. Hence,

$$\|A\|_F^2 = \|a\|^2 = \sum_{j=1}^s \|\alpha_j\|^2.$$

Therefore,

$$\|A\|_F^2 = \sum_{j=1}^s \|A_j\|_F^2. \quad (14)$$

On the other hand, it is clear that

$$\mathcal{E}(A_j) = \sum_{i=1}^{n_j} s_{ij}. \quad (15)$$

Furthermore, the description of $P(\lambda) = \det(A - \lambda I_n)$ in (12) makes it evident that

$$\mathcal{E}(A) = \sum_{j=1}^s \sum_{i=1}^{n_j} s_{ij} = \sum_{j=1}^s \mathcal{E}(A_j). \quad (16)$$

By considering the vectors $(1, \dots, 1)$ and $\alpha_j \in \mathbb{R}^{n_j}$ and by applying Cauchy Schwarz inequality on Eq. (15), we have

$$\mathcal{E}(A_j) \leq \sqrt{n_j} \|\alpha_j\| = \sqrt{n_j} \|A_j\|_F, \quad 1 \leq j \leq s. \quad (17)$$

Finally from Eqs. (16) and (17) we conclude that

$$\mathcal{E}(A) \leq \sum_{j=1}^s \sqrt{n_j} \|A_j\|_F.$$

Thus, the first inequality in (13) follows. It only remains to verify the second inequality in (13). We see that the following identity is immediate from the terminology introduced:

$$\|\varepsilon_{n_{t+1}}(\delta_{n_1+\dots+n_{t-1}+n_t}(a))\| = \|A_{t+1}\|_F, \quad 1 \leq t \leq s-1. \quad (18)$$

Using Lemma 1 we replace q by n , p by n_1 and considering Eqs. (14) and (18), we obtain

$$\sqrt{n_1} \|A_1\|_F + \sqrt{n - n_1} \|\delta_{n_1}(a)\| \leq \sqrt{n} \|a\| = \sqrt{n} \|A\|_F, \quad (19)$$

via $\|\varepsilon_{n_1}(a)\| = \|A_1\|_F$. We continue using Lemma 1, but this time we shall stick to change q to $n - n_1$, p to n_2 and a to $\delta_{n_1}(a) \in W^{n-n_1}$, together with Eq. (18) and the property **2**, we arrive to

$$\sqrt{n_2} \|A_2\|_F + \sqrt{n - n_1 - n_2} \|\delta_{n_2+n_1}(a)\| \leq \sqrt{n - n_1} \|\delta_{n_1}(a)\|, \quad (20)$$

via $\|\varepsilon_{n_2}(\delta_{n_1}(a))\| = \|A_2\|_F$. By considering Eqs. (19) and (20), we deduce that

$$\sqrt{n_1} \|A_1\|_F + \sqrt{n_2} \|A_2\|_F + \sqrt{n - n_1 - n_2} \|\delta_{n_2+n_1}(a)\| \leq \sqrt{n} \|A\|_F. \quad (21)$$

Using again Lemma 1 we replace q by $n - n_1 - n_2$, p by n_3 and a by $\delta_{n_2+n_1}(a) \in W^{n-n_2-n_1}$ and considering Eq. (18) and the above property **2**, we arrive to

$$\sqrt{n_3} \|A_3\|_F + \sqrt{n - n_1 - n_2 - n_3} \|\delta_{n_3+n_2+n_1}(a)\| \leq \sqrt{n - n_1 - n_2} \|\delta_{n_2+n_1}(a)\|, \quad (22)$$

via $\|\varepsilon_{n_3}(\delta_{n_2+n_1}(a))\| = \|A_3\|_F$. Eqs. (21) and (22) imply

$$\sqrt{n_1} \|A_1\|_F + \sqrt{n_2} \|A_2\|_F + \sqrt{n_3} \|A_3\|_F + \sqrt{n - n_1 - n_2 - n_3} \|\delta_{n_3+n_2+n_1}(a)\| \leq \sqrt{n} \|A\|_F.$$

If $s > 3$ we continue by applying the same kind of reasoning until to arrive to change in the inequality (7), q to $n - n_1 - n_2 - \dots - n_{s-2} = n_s + n_{s-1}$, p to n_{s-1} and a to $\delta_{n_{s-2}+n_{s-3}+\dots+n_1}(a) \in W^{n_s+n_{s-1}}$, to obtain

$$\sqrt{n_{s-1}} \|A_{s-1}\|_F + \sqrt{n_s} \|\delta_{n_{s-1}+n_{s-2}+\dots+n_1}(a)\|_F \leq \sqrt{n_s + n_{s-1}} \|\delta_{n_{s-2}+n_{s-3}+\dots+n_1}(a)\|_F,$$

via $\|\varepsilon_{n_{s-1}}(\delta_{n_{s-2}+n_{s-3}+\dots+n_1}(a))\|_F = \|A_{s-1}\|_F$. Then,

$$\sqrt{n_{s-1}} \|A_{s-1}\|_F + \sqrt{n_s} \|A_s\|_F \leq \sqrt{n_s + n_{s-1}} \|\delta_{n_{s-2}+n_{s-3}+\dots+n_1}(a)\|_F,$$

via $\|\delta_{n_{s-1}+n_{s-2}+\dots+n_1}(a)\|_F = \|A_s\|_F$. Therefore

$$\sqrt{n_1} \|A_1\|_F + \dots + \sqrt{n_{s-1}} \|A_{s-1}\|_F + \sqrt{n_s} \|A_s\|_F \leq$$

$$\sqrt{n_1} \|A_1\|_F + \dots + \sqrt{n_{s-2}} \|A_{s-2}\|_F + \sqrt{n_s + n_{s-1}} \|\delta_{n_{s-2}+n_{s-3}+\dots+n_1}(a)\|_F,$$

and

$$\sqrt{n_1} \|A_1\|_F + \dots + \sqrt{n_{s-2}} \|A_{s-2}\|_F + \sqrt{n_s + n_{s-1}} \|\delta_{n_{s-2}+n_{s-3}+\dots+n_1}(a)\|_F \leq \sqrt{n} \|A\|_F,$$

considering the previous step. This completes our argument. ■

Corollary 3 *Let G be an (n, m) -graph such that*

$$\det(L(G) - \lambda I_n) = P_1(\lambda) P_2(\lambda) \dots P_s(\lambda) \quad (23)$$

where $P_j(\lambda) = \det(A_j - \lambda I_j)$, where A_j are square matrices of order j with $1 \leq j \leq s$. Then

$$(LE)_G \leq \sum_{j=1}^s \sqrt{n_j} \|A_j - \frac{2m}{n} I_{n_j}\|_F \leq \sqrt{2Mn}, \quad (24)$$

where M is defined by (6).

Proof. From the decomposition of $\det(L(G) - \lambda I_n)$ in (23) (**) we see that

$$\begin{aligned} \det((L(G) - \frac{2m}{n} I_n) - \lambda I_n) &= \det(L(G) - (\frac{2m}{n} + \lambda) I_n) \\ &= P_1^o(\lambda) P_2^o(\lambda) \dots P_s^o(\lambda), \end{aligned}$$

where $P_j^o(\lambda) = \det(A_j - (\frac{2m}{n} + \lambda) I_{n_j})$. Using Theorem 2 we replace the matrix A by $L(G) - \frac{2m}{n} I_n$ and the matrices A_j by $A_j - \frac{2m}{n} I_{n_j}$ together with Eqs. (2) and (6), the expression in Eq. (24) follows. ■

Corollary 4 *Let G be an (n, m) -graph such that*

$$\det(L(G) - \lambda I_n) = P_1^{t_1}(\lambda) P_2^{t_2}(\lambda) \dots P_s^{t_s}(\lambda), \quad (25)$$

where $P_j(\lambda) = \det(A_j - \lambda I_j)$, where A_j are square matrices of order j with $1 \leq j \leq s$. Then

$$(LE)_G \leq \sum_{j=1}^s t_j \sqrt{n_j} \left\| A_j - \frac{2m}{n} I_{n_j} \right\|_F \leq \sqrt{2Mn}, \quad (26)$$

where M is defined by (6).

Proof. We consider Eq. (25) as

$$\det(L(G) - \lambda I_n) = (P_1(\lambda) \dots P_1(\lambda)) (P_2(\lambda) \dots P_2(\lambda)) \dots (P_s(\lambda) \dots P_s(\lambda)).$$

Therefore, using Corollary 3 we obtain

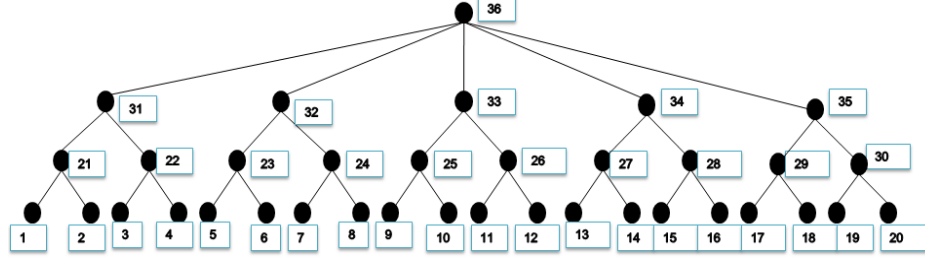
$$(LE)_G \leq \sum_{j=1}^s \sum_{|P_j|} \sqrt{n_j} \left\| A_j - \frac{2m}{n} I_{n_j} \right\|_F \leq \sqrt{2Mn},$$

where $|P_j|$ stands for the number of times that P_j is a factor of $\det(L(G) - \lambda I_n)$, namely t_j . Thus, the inequalities in (26) follow. ■

2 Improved upper bound for Laplacian energy of generalized Bethe trees

Let $k \geq 2$. A generalized Bethe tree B_k of k levels [12] is a rooted tree in which vertices at same level have the same degree. For $j = 1, \dots, k$, we denote by d_{k-j+1} and by n_{k-j+1} the degree of the vertices at level j and their number, respectively. Thus, $d_1 = 1$ is the degree of the vertices at the level k and d_k is the degree of the root vertex. Let $\mathbf{n} = (n_1, \dots, n_k)$. From now on we denote B_k by $B_k(\mathbf{n})$. In particular $B_k(\mathbf{n})$ is a bipartite graph. The following

figure illustrates the generalized Bethe tree $B_4(\mathbf{n})$ with $\mathbf{n} = (20, 10, 5, 1)$.



With the customary abuse of notation, we shall take n and m as the number of vertices and the number of edges of $B_k(\mathbf{n})$, respectively. Then, $m = n - 1$ and $\frac{2m}{n} = 2 - \frac{2}{n}$. The Laplacian energy of $B_k(\mathbf{n})$ is denoted by $(LE)_k$.

The aim of this section is to improve an upper bound for $(LE)_k$. On this way, we consider the tridiagonal symmetric matrix of order k

$$T_k = \begin{pmatrix} 1 & \sqrt{d_2 - 1} & & & \\ \sqrt{d_2 - 1} & d_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & & d_{k-1} & \sqrt{d_k} \\ & & & \sqrt{d_k} & d_k \end{pmatrix}.$$

For $1 \leq j \leq k - 1$, by setting T_j the corresponding principal leading submatrices of order j of T_k we consider the characteristic polynomials

$$P_j(\lambda) = \det(T_j - \lambda I_j), \quad 1 \leq j \leq k.$$

In addition let

$$\Phi = \{1, 2, \dots, k - 1\} \text{ and}$$

$$\Omega = \{j \in \Phi : n_j > n_{j+1}\}$$

and denote by a_j the integer

$$a_j = n_j - n_{j+1}, \quad 1 \leq j \leq k - 1.$$

The next result provides a split up of the characteristic polynomial of the Laplacian matrix.

Theorem 5 ([11]) For $1 \leq j \leq k$, let a_j, P_j be defined as above, respectively. Then the characteristic polynomial $P(\lambda) = \det(L(B_k(\mathbf{n})) - \lambda I_n)$ is decomposed in the form

$$P(\lambda) = P_k(\lambda) \prod_{j \in \Omega} P_j^{a_j}(\lambda).$$

By an application of Corollary 4 we obtain.

Theorem 6 For $1 \leq j \leq k$, let a_j, T_j be defined as above, respectively. Then

$$(LE)_k \leq \sqrt{k} \left\| T_k - \frac{2m}{n} I_k \right\|_F + \sum_{j \in \Omega} a_j \sqrt{j} \left\| T_j - \frac{2m}{n} I_j \right\|_F \leq \sqrt{2Mn}, \quad (27)$$

where M is defined by (6) with G replaced by $B_k(\mathbf{n})$.

Example 7 In what follows the vector \mathbf{n} is equal to the number of vertices of $B_k(\mathbf{n})$ labelled from bottom to top, the columns $(LE)_k$, OUB , NUB are the Laplacian energy, the upper bound obtained in [6], the upper bound obtained here, respectively.

\mathbf{n}	k	$(LE)_k$	OUB	NUB
(20, 10, 5, 1)	4	55.5044	64.0312	60.9150
(27, 9, 3, 1)	4	67.3657	78.4602	72.0270
(24, 12, 6, 3, 1)	5	70.3991	79.0696	76.4526
(64, 32, 16, 8, 4, 2, 1)	7	195.1063	219.0936	212.5950
(5, 1)	2	8.6667	11.8322	9.2326

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